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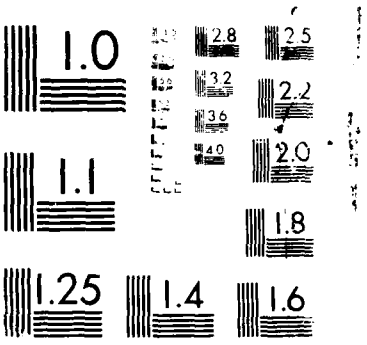

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Contract N00014-79-C-0648 involved the use of the experimental techniques thermal desorption spectroscopy (TDS), high resolution electron energy loss spectroscopy (HREELS) and low energy electron diffraction (LEED) and theoretical developments in the analysis of adsorbate vibrations to study the chemistry of a wide range of nitrogen containing hydrocarbons on transition metal surfaces. Fifteen technical reports resulted from the research.

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"VIBRATIONAL AND ELECTRONIC SPECTRA OF ADSORBED MOLECULES BY HIGH RESOLUTION ENERGY LOSS SPECTROSCOPY"

Contract #N00014-79-C-0648

FINAL REPORT

Principal Investigator: John C. Hemminger

FINAL REPORT

Contract N00014-79-C-0648 involved the use of the experimental techniques thermal desorption spectroscopy (TDS), high resolution electron energy loss spectroscopy (HREELS) and low energy electron diffraction (LEED) and theoretical developments in the analysis of adsorbate vibrations to study the chemistry of a wide range of nitrogen containing hydrocarbons on transition metal surfaces. Fifteen technical reports resulted from the research.

Experimental Results

The chemistry of several nitrogen containing hydrocarbons was examined in detail on a Pt(111) surface. These results indicate that cyanogen is often a stable product of the thermal decomposition of such compounds on Pt. In addition, cyanogen forms extremely stable films (stable to ~500°C) on Pt. These high temperature forms of cyanogen may be a two-dimensional "sheet" polymer which may prove to be an effective corrosion inhibition agent for transition metals. The detailed chemistry of these systems is described in technical reports 4, 6, 9, 13 and 15.

Several studies have also been carried out on the control of the ordering of molecules on surfaces by atomic scale defects. This work has indicated that ordered structures can be modified by the introduction of atomic scale defects into the substrate. This work is described in detail in technical reports 1, 2, 3 and 7.

Theory of Adsorbate Vibrations

A method for the analysis of adsorbate vibrations has been developed which is amenable to the study of molecular adsorbates including effects due to surface defects. This method utilizes clusters to describe the vibrations of the substrate

material. The method has been successfully applied to the problem of the damping of adsorbate vibrations by coupling to substrate phonons. The method was also used to investigate the sensitivity of isotope shifts of low frequency vibrations to adsorbate bonding site. This work is described in detail in technical reports 8, 10, 11, 12 and 14.

Technical Reports and Journal Articles

Contract No. N00014-79-C-0648

1. Symmetry Extinction of LEED Beams for Naphthalene Adsorbed on Pt(111).
   David Dahlgren and John C. Hemminger,
   Surface Science, 109, L513 (1981).

2. Chemisorption and Thermal Chemistry of Azulene and Naphthalene Adsorbed on Pt(111).
   David Dahlgren and John C. Hemminger,
   Surface Science, 114, 459 (1982).

3. The Nature of the Phase Transition Observed for Monolayers of Azulene on Pt(111).
   David Dahlgren and John C. Hemminger,
   J. Chem. Phys., 75, 5573 (1981).

4. The Chemistry of Dimethyltetrazine on Pt(111).
   David Dahlgren and John C. Hemminger,
   Surface Science, 120, 456 (1982).

5. Control of the UTI 100C Quadrupole Mass Spectrometer with an Inexpensive Microcomputer.
   David Dahlgren, John Arnold, and John C. Hemminger,
   J. Vac. Sci. Tech. A, 1, 81 (1983).

6. Decomposition of NO_2 to NO and O on Pt(111).
   David Dahlgren and John C. Hemminger,
   Surface Science, 123, 1739 (1983).

7. Chemisorption and Ordering of Naphthalene and Azulene on Pt(S) [7(111) x (100)]: The Effect of Periodic Defects on Long Range Order.
   David Dahlgren and John C. Hemminger,
   Surface Science, 134, 836 (1983).

8. Anharmonic Damping of Adsorbate Vibrational Modes.
   J.C. Ariyasu, D.L. Mills, Kathryn G. Lloyd, and John C. Hemminger,
   Physical Review B, 28, 6123 (1983).

9. Coadsorption Chemistry of H_2 and C_2N_2 on Pt(111): A Common Intermediate in the Hydrogenation of Cyanogen and the Dehydrogenation of Ethylenediamine on Pt(111).
   J.R. Kingsley, David Dahlgren and John C. Hemminger,
   Surface Science, 139, 417 (1984).

10. Cluster Analysis of the p(2x2) Oxygen Structure on Ni(100).
Kathryn G. Lloyd and John C. Hemminger,
Surface Science, 143, 509 (1984).

11. The Lifetime of Adsorbate Vibrations: The Role of Anharmonicity.
J.C. Ariyasu, D.L. Mills, Kathryn G. Lloyd, and John C. Hemminger,
Physical Review B, 30, 507 (1984).

12. A Cluster Approach to the Analysis of Adsorbate Vibrations.
Kathryn G. Lloyd and John C. Hemminger,
J. Chem. Phys., 82, 3858 (1985).

13. Generation of Cyanogen from the Decomposition of Several Nitrogen Containing Aromatics on Pt(111).
J.R. Kingsley and J.C. Hemminger,
Langmuir, 2, 460 (1986).

14. Vibrational Analysis of Water Adsorbed on Pd(100): Sensitivity of the Isotope Shifts of Bending Modes to the Binding Site.
Kathryn G. Lloyd, Barbara Banse, and John C. Hemminger,
Physical Review B, 33(4) 2858 (1986).

15. A HREELS/TDS Study of the Intermediate Formed by the Reaction of C_2N_2 with H_2 on Pt(111).
Kathryn G. Lloyd and John C. Hemminger,
Surface Science, 179, L6 (1987).

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